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Mn K-edge XANES of $Pr_{1-x}Ca_xMnO_3$ Colossal Magnetoresistive Manganites

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Beamline(s): X19A

Introduction: The major focus of CMR research has been on the "metallic" manganites with relatively broad bandwidths and $T_c \sim T_{mi}$. $Pr_{1-x}Ca_xMnO_3$ (x~0.3) exhibits unusual physical properties, including a charge order transition before the ferromagnetic transition transition, $T_c \neq T_{mi}$, and a x-ray photoinduced meal-insulator (MI) transition at low temperature [1] which are believed to be due to a narrow bandwidth controlled through the distortions from the perfect MnO_6 octahedra. The local structure at low temperatures and local structure transformations under exposure to intense synchrotron x-rays are of significant interest.

Methods and Materials: The $Pr_{1-x}Ca_xMnO_3$ family is a challenge for Mn *K*-edge x-ray absorption measurements. In contrast to $La_{1-x}Ca_xMnO_3$ where the Mn *K*-edge follows all La edges, in $Pr_{0.7}Ca_{0.3}MnO_3$ the Mn *K*-edge (E=6.54 KeV) lies between the Pr L_3-(E=6.44 KeV) and Pr L_2-(E=6.84 KeV) edges (Fig. 1). Fluorescent yield (FY) detection *alone* does not help since an inverted edge appears at E~ 6.84 KeV due to a jump in the self-absorption coefficient. As a result, the XAFS range in k-space is too short to obtain any reliable information about local structural distortions. If data is are collected in a transmission mode (TM), than even quantitative analysis of the XANES appears not to be straight forward: large residual oscillations from Pr L_3 edge distort details of the fine structure at the Mn *K*-edge.

Results: We proposed correction in both XANES and EXAFS areas.

XANES spectrum. Mn K_α FY detection can strongly reduce the contribution from the Pr L_3-edge. The reduction is due to: (i) three times larger FY at the Mn *K*- than that at Pr L_3 edge and (ii) an energy window of multi-element Ge detector is placed at ~100-150 eV above the Mn K_α line. Though the suppression is not complete, at least 10 times improvement other the TM case can be easily achieved at the high-flux beamline X19a (Fig. 1). We have investigated Mn *K*-edge XANES of $Pr_{1-x}Ca_xMnO_3$ as a function Ca doping for x=0.1, 0.2, 0.3, 0.4, and 0.5 at 120 and 300K.

XAFS spectrum. Two experimental EXAFS spectra (collected simultaneously in TM and FY modes) are enable one to restore an absorption coefficient at the Mn *K*- edge, $\mu(E)$, using a well-known relation for the self-absorption correction. In the case of a thick sample the normalized fluorescent intensity (I_f) with the background (I_b) subtracted is given by: $I_f - I_B \propto \mu(E)/(\mu_{tot}(E) + \mu_{tot}(E_f)g)$ Here g characterizes the detection geometry, and $\mu_{tot}(E)$, is the total absorption coefficient. It is an essential advantage of the proposed approach that the $\mu_{tot}(E)$ is taken from direct XAFS measurements in TM, and, therefore, it involves all multiple scattering contributions and the genuine background behavior. For a concentrated sample, the signal-to-noise ratio in the TM measurements is basically much larger than in the FY mode, so that noise in the TM data is only slightly affects the result of the math correction. Other corrections to be applied to the raw data are the following: (i) background correction in the FY measurements; (ii) correction for different energy resolution in TM and FY; (iii) correction for different geometry of individual Ge detectors; (iv) correction for energy-dependent transparency of the ion chamber(s). Our preliminary results [2] demonstrated a potential for reconstructing the $k\chi(k)$ XAFS of reasonably good quality up to 10-11Å^{-1}.

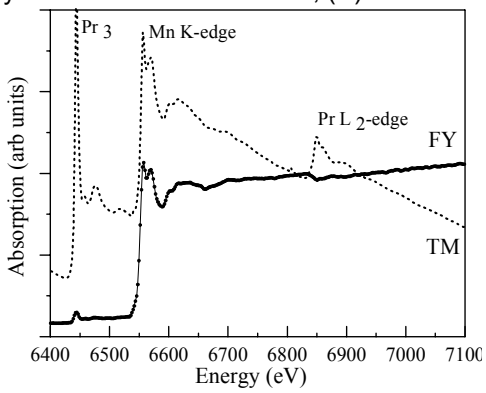

Fig. 1. Raw experimental data of $Pr_{0.7}Ca_{0.3}MnO_3$ collected at X19a simultaneously in FY and TM at 120 K. FY spectrum was obtained as described in the text.

Conclusions: We have developed and tested a procedure allowing one to expand the Mn *K*-edge EXAFS spectra above the Pr L_3- edge in $Pr_{0.7}Ca_{0.3}MnO_3$. Importantly, it has much more general applicability: There are many magnetic materials involving *3d* metals and rare earths whose XAFS analyses are currently not possible due to interference of edges. Further improvements of the correction procedures and the advent of the third-generation synchrotron light sources as well as the appearance of new fluorescence detectors will open the road for such studies.

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References:

[1] V. Kiryukhin *et al*., *Nature* **386**, 813 (1997).

[2] A. Ignatov *et al*., *XAFS-XI*, Japan, 2000 (unpublished).